Finite difference methods for diffusion processes

Hans Petter Langtangen[1,2]

[1]Center for Biomedical Computing, Simula Research Laboratory
[2]Department of Informatics, University of Oslo

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Contents

1 The 1D diffusion equation

The famous *diffusion equation*, also known as the *heat equation*, reads

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2},$$

where $u(x,t)$ is the unknown function to be solved for, x is a coord space, and t is time. The coefficient α is the *diffusion coefficient* and det how fast u changes in time. A quick short form for the diffusion equ $u_t = \alpha u_{xx}$.

Compared to the wave equation, $u_{tt} = c^2 u_{xx}$, which looks very simi the diffusion equation features solutions that are very different from thos wave equation. Also, the diffusion equation makes quite different dem the numerical methods.

Typical diffusion problems may experience rapid change in the very be but then the evolution of u becomes slower and slower. The solution is very smooth, and after some time, one cannot recognize the initial sha This is in sharp contrast to solutions of the wave equation where the initi is preserved - the solution is basically a moving initial condition. The s wave equation $u_{tt} = c^2 u_{xx}$ has solutions that propagates with speed c without changing shape, while the diffusion equation converges to a *st solution* $\bar{u}(x)$ as $t \to \infty$. In this limit, $u_t = 0$, and $\bar{u}$ is governed by $\bar{u}''$ This stationary limit of the diffusion equation is called the *Laplace* equat arises in a very wide range of applications throughout the sciences.

It is possible to solve for $u(x,t)$ using a explicit scheme, but the ti restrictions soon become much less favorable than for an explicit scheme wave equation. And of more importance, since the solution u of the d equation is very smooth and changes slowly, small time steps are not co and not required by accuracy as the diffusion process converges to a st state.

1.1 The initial-boundary value problem for 1D diffu

To obtain a unique solution of the diffusion equation, or equivalently, t numerical methods, we need initial and boundary conditions. The d equation goes with one initial condition $u(x,0) = I(x)$, where I is a pr function. One boundary condition is required at each point on the ary, which in 1D means that u must be known, u_x must be known, combination of them.

We shall start with the simplest boundary condition: $u = 0$. The complete itial-boundary value diffusion problem in one space dimension can then be ecified as

$$\frac{\partial u}{\partial t} = \alpha \frac{\partial^2 u}{\partial x^2}, \quad x \in (0, L),\ t \in (0, T] \tag{1}$$

$$u(x, 0) = I(x), \qquad x \in [0, L] \tag{2}$$

$$u(0, t) = 0, \qquad t > 0, \tag{3}$$

$$u(L, t) = 0, \qquad t > 0\,. \tag{4}$$

quation (64) is known as a one-dimensional *diffusion equation*, also often eferred to as a *heat equation*. With only a first-order derivative in time, only ne *initial condition* is needed, while the second-order derivative in space leads o a demand for two *boundary conditions*. The parameter α must be given and referred to as the *diffusion coefficient*.

Diffusion equations like (64) have a wide range of applications throughout hysical, biological, and financial sciences. One of the most common applications propagation of heat, where $u(x, t)$ represents the temperature of some substance t point x and time t. Section **??** goes into several widely occurring applications.

.2 Forward Euler scheme

he first step in the discretization procedure is to replace the domain $[0, L]\times[0, T]$ y a set of mesh points. Here we apply equally spaced mesh points

$$x_i = i\Delta x, \quad i = 0, \ldots, N_x,$$

nd

$$t_n = n\Delta t, \quad n = 0, \ldots, N_t\,.$$

Ioreover, u_i^n denotes the mesh function that approximates $u(x_i, t_n)$ for $i = , \ldots, N_x$ and $n = 0, \ldots, N_t$. Requiring the PDE (64) to be fulfilled at a mesh oint (x_i, t_n) leads to the equation

$$\frac{\partial}{\partial t} u(x_i, t_n) = \alpha \frac{\partial^2}{\partial x^2} u(x_i, t_n), \tag{5}$$

he next step is to replace the derivatives by finite difference approximations. he computationally simplest method arises from using a forward difference in me and a central difference in space:

$$[D_t^+ u = \alpha D_x D_x u]_i^n\,. \tag{6}$$

/ritten out,

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}\,. \tag{7}$$

We have turned the PDE into algebraic equations, also often called equations. The key property of the equations is that they are algebraic makes them easy to solve. As usual, we anticipate that u_i^n is already co such that u_i^{n+1} is the only unknown in (7). Solving with respect to this u is easy:

$$u_i^{n+1} = u_i^n + Fo\left(u_{i+1}^n - 2u_i^n + u_{i-1}^n\right),$$

where we have introduced the *mesh Fourier number*

$$Fo = \alpha \frac{\Delta t}{\Delta x^2}\,.$$

Fo is the key parameter in the discrete diffusion equation.

Note that Fo is a *dimensionless* number that lumps the key phy parameter in the problem, α, and the discretization parameters Δx Δt into a single parameter. All the properties of the numerical metho critically dependent upon the value of Fo (see Section 2.3 for details

The computational algorithm then becomes

1. compute $u_i^0 = I(x_i)$for $i = 0, \ldots, N_x$
2. for $n = 0, 1, \ldots, N_t$:
   (a) apply (8) for all the internal spatial points $i = 1, \ldots, N_x - 1$
   (b) set the boundary values $u_i^{n+1} = 0$ for $i = 0$ and $i = N_x$

The algorithm is compactly fully specified in Python:

```
x = linspace(0, L, Nx+1)    # mesh points in space
dx = x[1] - x[0]
t = linspace(0, T, Nt+1)    # mesh points in time
dt = t[1] - t[0]
Fo = a*dt/dx**2
u   = zeros(Nx+1)
u_1 = zeros(Nx+1)

# Set initial condition u(x,0) = I(x)
for i in range(0, Nx+1):
    u_1[i] = I(x[i])

for n in range(0, Nt):
    # Compute u at inner mesh points
    for i in range(1, Nx):
        u[i] = u_1[i] + Fo*(u_1[i-1] - 2*u_1[i] + u_1[i+1])

    # Insert boundary conditions
    u[0] = 0;  u[Nx] = 0
```

```
# Update u_1 before next step
u_1[:]= u
```

The program `diffu1D_u0.py`[1] contains a function `solver_FE` for solving ıe 1D diffusion equation with $u = 0$ on the boundary. The functions `plug` ıd `gaussian` runs the case with $I(x)$ as a discontinuous plug or a smooth aussian function, respectively. Experiments with these two functions reveal ome important observations:

- The Forward Euler scheme leads to growing solutions if $Fo > \frac{1}{2}$.
- $I(x)$ as a discontinuous plug leads to a saw tooth-like noise for $Fo = \frac{1}{2}$, see movie[2], which is absent for $Fo \leq \frac{1}{4}$, see movie[3].
- The smooth Gaussian initial function leads to a smooth solution, see movie[4] for $Fo = \frac{1}{2}$.

.3 Backward Euler scheme

/e now apply a backward difference in time in (5), but the same central difference ı space:

$$[D_t^- u = D_x D_x u]_i^n, \tag{10}$$

hich written out reads

$$\frac{u_i^n - u_i^{n-1}}{\Delta t} = \alpha \frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}\,. \tag{11}$$

ow we assume u_i^{n-1} is computed, but all quantities at the "new" time level n re unknown. This time it is not possible to solve with respect to u_i^n because this alue couples to its neighbors in space, u_{i-1}^n and u_{i+1}^n, which are also unknown. et us examine this fact for the case when $N_x = 3$. Equation (11) written for $= 1, \ldots, Nx - 1 = 1, 2$ becomes

$$\frac{u_1^n - u_1^{n-1}}{\Delta t} = \alpha \frac{u_2^n - 2u_1^n + u_0^n}{\Delta x^2} \tag{12}$$

$$\frac{u_2^n - u_2^{n-1}}{\Delta t} = \alpha \frac{u_3^n - 2u_2^n + u_1^n}{\Delta x^2} \tag{13}$$

he boundary values u_0^n and u_3^n are known as zero. Collecting the unknown new alues u_1^n and u_2^n on the left-hand side gives

[1] `http://tinyurl.com/jvzzcfn/diffu/diffu1D_u0.py`
[2] `http://tinyurl.com/k3sdbuv/pub/mov-diffu/diffu1D_u0_FE_plug/movie.ogg`
[3] `http://tinyurl.com/k3sdbuv/pub/mov-diffu/diffu1D_u0_FE_plug_Fo025/movie.ogg`
[4] `http://tinyurl.com/k3sdbuv/pub/mov-diffu/diffu1D_u0_FE_plug_gaussian1/movie.ogg`

$$(1 + 2Fo)\, u_1^n - Fou_2^n = u_1^{n-1},$$
$$-Fou_1^n + (1 + 2Fo)\, u_2^n = u_2^{n-1}\,.$$

This is a coupled 2×2 system of algebraic equations for the unknowns u_2^n. The equivalent matrix form is

$$\begin{pmatrix} 1 + 2Fo & -Fo \\ -Fo & 1 + 2Fo \end{pmatrix} \begin{pmatrix} u_1^n \\ u_2^n \end{pmatrix} = \begin{pmatrix} u_1^{n-1} \\ u_2^{n-1} \end{pmatrix}$$

Implicit vs. explicit methods.

Discretization methods that lead to a coupled system of equations fo unknown function at a new time level are said to be *implicit methods*. counterpart, *explicit methods*, refers to discretization methods where is a simple explicit formula for the values of the unknown function at of the spatial mesh points at the new time level. From an implementat point of view, implicit methods are more comprehensive to code since require the solution of coupled equations, i.e., a matrix system, at time level.

In the general case, (11) gives rise to a coupled $(Nx - 1) \times (Nx - 1)$ of algebraic equations for all the unknown u_i^n at the interior spatia $i = 1, \ldots, Nx - 1$. Collecting the unknowns on the left-hand side, (11) written

$$-F_o u_{i-1}^n + (1 + 2F_o)\, u_i^n - F_o u_{i+1}^n = u_{i-1}^{n-1},$$

for $i = 1, \ldots, Nx - 1$. One can either view these equations as a system fc the u_i^n values at the internal mesh points, $i = 1, \ldots, N_x - 1$, are unknow may append the boundary values u_0^n and $u_{N_x}^n$ to the system. In the lat all u_i^n for $i = 0, \ldots, N_x$ are unknown and we must add the boundary ec to the $N_x - 1$ equations in (16):

$$u_0^n = 0,$$
$$u_{N_x}^n = 0\,.$$

A coupled system of algebraic equations can be written on matr and this is important if we want to call up ready-made software for solv system. The equations (16) and (17)–(18) correspond to the matrix eq

$$AU = b$$

where $U = (u_0^n, \ldots, u_{N_x}^n)$, and the matrix A has the following structure

$$
= \begin{pmatrix}
A_{0,0} & A_{0,1} & 0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 \\
A_{1,0} & A_{1,1} & 0 & \ddots & & & & & \vdots \\
0 & A_{2,1} & A_{2,2} & A_{2,3} & \ddots & & & & \vdots \\
\vdots & \ddots & & \ddots & \ddots & 0 & & & \vdots \\
\vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & & \vdots \\
\vdots & & & 0 & A_{i,i-1} & A_{i,i} & A_{i,i+1} & \ddots & \vdots \\
\vdots & & & & \ddots & \ddots & \ddots & \ddots & 0 \\
\vdots & & & & & \ddots & \ddots & \ddots & A_{N_x-1,N_x} \\
0 & \cdots & \cdots & \cdots & \cdots & \cdots & 0 & A_{N_x,N_x-1} & A_{N_x,N_x}
\end{pmatrix} \tag{19}
$$

he nonzero elements are given by

$$A_{i,i-1} = -F_o \tag{20}$$
$$A_{i,i} = 1 + 2F_o \tag{21}$$
$$A_{i,i+1} = -F_o \tag{22}$$

or the equations for internal points, $i = 1, \ldots, N_x - 1$. The equations for the oundary points correspond to

$$A_{0,0} = 1, \tag{23}$$
$$A_{0,1} = 0, \tag{24}$$
$$A_{N_x,N_x-1} = 0, \tag{25}$$
$$A_{N_x,N_x} = 1\,. \tag{26}$$

he right-hand side b is written as

$$b = \begin{pmatrix} b_0 \\ b_1 \\ \vdots \\ b_i \\ \vdots \\ b_{N_x} \end{pmatrix} \tag{27}$$

ith

$$b_0 = 0, \tag{28}$$
$$b_i = u_i^{n-1}, \quad i = 1, \ldots, N_x - 1, \tag{29}$$
$$b_{N_x} = 0\,. \tag{30}$$

We observe that the matrix A contains quantities that do not ch time. Therefore, A can be formed once and for all before we enter the r formulas for the time evolution. The right-hand side b, however, must be at each time step. This leads to the following computational algorith sketched with Python code:

```
x = linspace(0, L, Nx+1)   # mesh points in space
dx = x[1] - x[0]
t = linspace(0, T, N+1)    # mesh points in time
u   = zeros(Nx+1)
u_1 = zeros(Nx+1)

# Data structures for the linear system
A = zeros((Nx+1, Nx+1))
b = zeros(Nx+1)

for i in range(1, Nx):
    A[i,i-1] = -Fo
    A[i,i+1] = -Fo
    A[i,i] = 1 + 2*Fo
A[0,0] = A[Nx,Nx] = 1

# Set initial condition u(x,0) = I(x)
for i in range(0, Nx+1):
    u_1[i] = I(x[i])

import scipy.linalg

for n in range(0, Nt):
    # Compute b and solve linear system
    for i in range(1, Nx):
        b[i] = -u_1[i]
    b[0] = b[Nx] = 0
    u[:] = scipy.linalg.solve(A, b)

    # Update u_1 before next step
    u_1[:] = u
```

1.4 Sparse matrix implementation

We have seen from (19) that the matrix A is tridiagonal. The code s above used a full, dense matrix representation of A, which stores a lot o we know are zero beforehand, and worse, the solution algorithm compu all these zeros. With $N_x + 1$ unknowns, the work by the solution algo $\frac{1}{3}(N_x + 1)^3$ and the storage requirements $(N_x + 1)^2$. By utilizing the fact is tridiagonal and employing corresponding software tools, the work and demands can be proportional to N_x only.

The key idea is to apply a data structure for a tridiagonal or sparse The `scipy.sparse` package has relevant utilities. For example, we can s nonzero diagonals of a matrix. The package also has linear system solv operate on sparse matrix data structures. The code below illustrates can store only the main diagonal and the upper and lower diagonals.

```
# Representation of sparse matrix and right-hand side
main  = zeros(Nx+1)
lower = zeros(Nx-1)
upper = zeros(Nx-1)
b     = zeros(Nx+1)

# Precompute sparse matrix
main[:] = 1 + 2*Fo
lower[:] = -Fo  #1
upper[:] = -Fo  #1
# Insert boundary conditions
main[0] = 1
main[Nx] = 1

A = scipy.sparse.diags(
    diagonals=[main, lower, upper],
    offsets=[0, -1, 1], shape=(Nx+1, Nx+1),
    format='csr')
print A.todense()  # Check that A is correct

# Set initial condition
for i in range(0,Nx+1):
    u_1[i] = I(x[i])

for n in range(0, Nt):
    b = u_1
    b[0] = b[-1] = 0.0  # boundary conditions
    u[:] = scipy.sparse.linalg.spsolve(A, b)
    u_1[:] = u
```

The `scipy.sparse.linalg.spsolve` function utilizes the sparse storage structure of `A` and performs in this case a very efficient Gaussian elimination solve.

The program `diffu1D_u0.py`[5] contains a function `solver_BE`, which implements the Backward Euler scheme sketched above. As mentioned in Section 1.2, the functions `plug` and `gaussian` runs the case with $I(x)$ as a discontinuous plug or a smooth Gaussian function. All experiments point to two characteristic features of the Backward Euler scheme: 1) it is always stable, and 2) it always gives a smooth, decaying solution.

.5 Crank-Nicolson scheme

The idea in the Crank-Nicolson scheme is to apply centered differences in space and time, combined with an average in time. We demand the PDE to be fulfilled at the spatial mesh points, but in between the points in the time mesh:

$$\frac{\partial}{\partial t}u(x_i, t_{n+\frac{1}{2}}) = \alpha\frac{\partial^2}{\partial x^2}u(x_i, t_{n+\frac{1}{2}}).$$

for $i = 1, \ldots, N_x - 1$ and $n = 0, \ldots, N_t - 1$.

With centered differences in space and time, we get

$$[D_t u = \alpha D_x D_x u]_i^{n+\frac{1}{2}}\,.$$

[5] `http://tinyurl.com/jvzzcfn/diffu/diffu1D_u0.py`

On the right-hand side we get an expression

$$u_{i-1}^{n+\frac{1}{2}} - u_i^{n+\frac{1}{2}} + u_{i+1}^{n+\frac{1}{2}}\,.$$

This is problematic since $u_i^{n+\frac{1}{2}}$ is not one of the unknown we comp possibility is to replace $u_i^{n+\frac{1}{2}}$ by an arithmetic average:

$$u_i^{n+\frac{1}{2}} \approx \frac{1}{2}\left(u_i^n + u_i^{n+1}\right)\,.$$

In the compact notation, we can use the arithmetic average notation $\overline{u}^t$

$$[D_t u = \alpha D_x D_x \overline{u}^t]_i^{n+\frac{1}{2}}\,.$$

After writing out the differences and average, multiplying by Δt, and ing all unknown terms on the left-hand side, we get

$$u_i^{n+1} - \frac{1}{2}Fo(u_{i-1}^{n+1} - 2u_i^{n+1} + u_{i+1}^{n+1}) = u_i^n + \frac{1}{2}Fo(u_{i-1}^n - 2u_i^n + u_{i+1}^n)$$

Also here, as in the Backward Euler scheme, the new unknowns u_{i-}^{n+} and u_{i+1}^{n+1} are coupled in a linear system $AU = b$, where A has the same s as in (19), but with slightly different entries:

$$\begin{aligned} A_{i,i-1} &= -\frac{1}{2}F_o \\ A_{i,i} &= \frac{1}{2} + F_o \\ A_{i,i+1} &= -\frac{1}{2}F_o \end{aligned}$$

for the equations for internal points, $i = 1, \ldots, N_x - 1$. The equations boundary points correspond to

$$\begin{aligned} A_{0,0} &= 1, \\ A_{0,1} &= 0, \\ A_{N_x,N_x-1} &= 0, \\ A_{N_x,N_x} &= 1\,. \end{aligned}$$

The right-hand side b has entries

$$\begin{aligned} b_0 &= 0, \\ b_i &= u_i^{n-1}, \quad i = 1, \ldots, N_x - 1, \\ b_{N_x} &= 0\,. \end{aligned}$$

.6 The θ rule

he θ rule provides a family of finite difference approximations in time:

- $\theta = 0$ gives the Forward Euler scheme in time
- $\theta = 1$ gives the Backward Euler scheme in time
- $\theta = \frac{1}{2}$ gives the Crank-Nicolson scheme in time

pplied to the 1D diffusion problem we have

$$\frac{u_i^{n+1} - u_i^n}{\Delta t} = \alpha \left(\theta \frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{\Delta x^2} + (1-\theta)\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2} \right).$$

his scheme also leads to a matrix system with entries

$$A_{i,i-1} = -F_o\theta, \quad A_{i,i} = 1 + 2F_o\theta \quad , A_{i,i+1} = -F_o\theta,$$

hile right-hand side entry b_i is

$$b_i = u_i^n + F_o(1-\theta)\frac{u_{i+1}^n - 2u_i^n + u_{i-1}^n}{\Delta x^2}$$

he corresponding entries for the boundary points are as in the Backward Euler nd Crank-Nicolson schemes listed earlier.

.7 The Laplace and Poisson equation

he Laplace equation, $\nabla^2 u = 0$, or the Poisson equation, $-\nabla^2 u = f$, occur in umerous applications throughout science and engineering. In 1D these equations ead $u''(x) = 0$ and $-u''(x) = f(x)$, respectively. We can solve 1D variants of ne Laplace equations with the listed software, because we can interpret $u_{xx} = 0$ s the limiting solution of $u_t = \alpha u_{xx}$ when u reach a steady state limit where $_t \to 0$. Similarly, Poisson's equation $-u_{xx} = f$ arises from solving $u_t = u_{xx} + f$ nd letting $t \to$ so $u_t \to 0$.

Technically in a program, we can simulate $t \to \infty$ by just taking one large me step, or equivalently, set α to a large value. All we need is to have F_o large. s $F_o \to \infty$, we can from the schemes see that the limiting discrete equation ecomes

$$\frac{u_{i+1}^{n+1} - 2u_i^{n+1} + u_{i-1}^{n+1}}{\Delta x^2} = 0,$$

hich is nothing but the discretization $[D_x D_x u]_i^{n+1} = 0$ of $u_{xx} = 0$.

The Backward Euler scheme can solve the limit equation directly and hence roduce a solution of the 1D Laplace equation. With the Forward Euler scheme e must do the time stepping since $F_o > 1/2$ is illegal and leads to instability. /e may interpret this time stepping as solving the equation system from u_{xx} by erating on a time pseudo time variable.

1.8 Extensions

These extensions are performed exactly as for a wave equation as they on the spatial derivatives (which are the same as in the wave equation).

- Variable coefficients
- Neumann and Robin conditions
- 2D and 3D

Future versions of this document will for completeness and independenc wave equation document feature info on the three points. The Robin cc is new, but straightforward to handle:

$$-\alpha\frac{\partial u}{\partial n} = h_T(u - U_s), \quad [-\alpha D_x u = h_T(u - U_s)]_i^n$$

2 Analysis of schemes for the diffusion equ

2.1 Properties of the solution

A particular characteristic of diffusive processes, governed by an equati

$$u_t = \alpha u_{xx},$$

is that the initial shape $u(x,0) = I(x)$ spreads out in space with tim with a decaying amplitude. Three different examples will illustrate the sp of u in space and the decay in time.

Similarity solution. The diffusion equation (42) admits solutions that on $\eta = (x-c)/\sqrt{4\alpha t}$ for a given value of c. One particular solution is

$$u(x,t) = a\,\mathrm{erf}(\eta) + b,$$

where

$$\mathrm{erf}(\eta) = \frac{2}{\sqrt{\pi}}\int_0^\eta e^{-\zeta^2}d\zeta,$$

is the *error function*, and a and b are arbitrary constants. The error f lies in $(-1,1)$, is odd around $\eta = 0$, and goes relatively quickly to ± 1:

$$\lim_{\eta\to-\infty}\text{erf}(\eta) = -1,$$
$$\lim_{\eta\to\infty}\text{erf}(\eta) = 1,$$
$$\text{erf}(\eta) = -\text{erf}(-\eta),$$
$$\text{erf}(0) = 0,$$
$$\text{erf}(2) = 0.99532227,$$
$$\text{erf}(3) = 0.99997791\,.$$

As $t \to 0$, the error function approaches a step function centered at $x = c$. or a diffusion problem posed on the unit interval $[0,1]$, we may choose the step t $x = 1/2$ (meaning $c = 1/2$), $a = -1/2$, $b = 1/2$. Then

$$u(x,t) = \frac{1}{2}\left(1 - \text{erf}\left(\frac{x-\frac{1}{2}}{\sqrt{4\alpha t}}\right)\right) = \frac{1}{2}\text{erfc}\left(\frac{x-\frac{1}{2}}{\sqrt{4\alpha t}}\right), \tag{45}$$

here we have introduced the *complementary error function* $\text{erfc}(\eta) = 1 - \text{erf}(\eta)$. he solution (45) implies the boundary conditions

$$u(0,t) = \frac{1}{2}\left(1 - \text{erf}\left(\frac{-1/2}{\sqrt{4\alpha t}}\right)\right), \tag{46}$$
$$u(1,t) = \frac{1}{2}\left(1 - \text{erf}\left(\frac{1/2}{\sqrt{4\alpha t}}\right)\right). \tag{47}$$

or small enough t, $u(0,t) \approx 1$ and $u(1,t) \approx 1$, but as $t \to \infty$, $u(x,t) \to 1/2$ on), 1].

olution for a Gaussian pulse. The standard diffusion equation $u_t = \alpha u_{xx}$ dmits a Gaussian function as solution:

$$u(x,t) = \frac{1}{\sqrt{4\pi\alpha t}}\exp\left(-\frac{(x-c)^2}{4\alpha t}\right). \tag{48}$$

t $t = 0$ this is a Dirac delta function, so for computational purposes one must art to view the solution at some time $t = t_\epsilon > 0$. Replacing t by $t_\epsilon + t$ in 8) makes it easy to operate with a (new) t that starts at $t = 0$ with an initial ondition with a finite width. The important feature of (48) is that the standard eviation σ of a sharp initial Gaussian pulse increases in time according to $= \sqrt{2\alpha t}$, making the pulse diffuse and flatten out.

olution for a sine component. For example, (42) admits a solution of the rm

$$u(x,t) = Qe^{-at}\sin(kx)\,. \tag{49}$$

The parameters Q and k can be freely chosen, while inserting (49) in (4 the constraint

$$a = -\alpha k^2\,.$$

A very important feature is that the initial shape $I(x) = Q\sin kx$ ur a damping $\exp(-\alpha k^2 t)$, meaning that rapid oscillations in space, corres to large k, are very much faster dampened than slow oscillations i corresponding to small k. This feature leads to a smoothing of th condition with time.

The following examples illustrates the damping properties of (4 consider the specific problem

$$u_t = u_{xx}, \quad x \in (0,1),\ t \in (0,T],$$
$$u(0,t) = u(1,t) = 0, \quad t \in (0,T],$$
$$u(x,0) = \sin(\pi x) + 0.1\sin(100\pi x)\,.$$

The initial condition has been chosen such that adding two solutions l constructs an analytical solution to the problem:

$$u(x,t) = e^{-\pi^2 t}\sin(\pi x) + 0.1e^{-\pi^2 10^4 t}\sin(100\pi x)\,.$$

Figure 1 illustrates the rapid damping of rapid oscillations $\sin(100\pi x)$ very much slower damping of the slowly varying $\sin(\pi x)$ term. Afte $t = 0.5\cdot 10^{-4}$ the rapid oscillations do not have a visible amplitude, w have to wait until $t \sim 0.5$ before the amplitude of the long wave $\sin(\pi x)$ l very small.

2.2 Analysis of discrete equations

A counterpart to (49) is the complex representation of the same functic

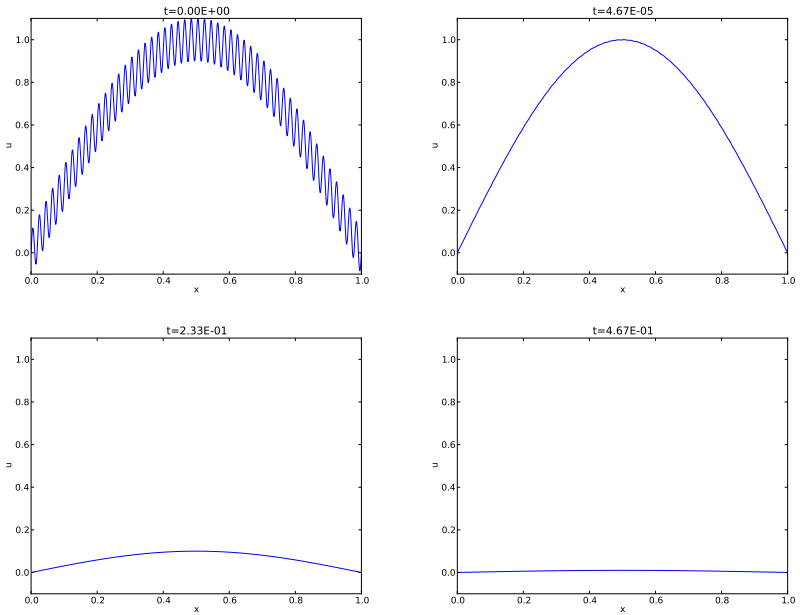
$$u(x,t) = Qe^{-at}e^{ikx},$$

where $i = \sqrt{-1}$ is the imaginary unit. We can add such functions, often to as wave components, to make a Fourier representation of a general sol the diffusion equation:

$$u(x,t) \approx \sum_{k\in K} b_k e^{-\alpha k^2 t}e^{ikx},$$

where K is a set of an infinite number of k values needed to constr solution. In practice, however, the series is truncated and K is a finite values need build a good approximate solution. Note that (50) is a spec of (51) where $K = \{\pi, 100\pi\}$, $b_\pi = 1$, and $b_{100\pi} = 0.1$.

The amplitudes b_k of the individual Fourier waves must be determin the initial condition. At $t = 0$ we have $u \approx \sum_k b_k \exp(ikx)$ and find K such that



igure 1: Evolution of the solution of a diffusion problem: initial condition
ıpper left), 1/100 reduction of the small waves (upper right), 1/10 reduction of
ıe long wave (lower left), and 1/100 reduction of the long wave (lower right).

$$I(x) \approx \sum_{k \in K} b_k e^{ikx}\,. \tag{52}$$

The relevant formulas for b_k come from Fourier analysis, or equivalently, a
east-squares method for approximating $I(x)$ in a function space with basis
$\exp(ikx)$.)

Much insight about the behavior of numerical methods can be obtained by
ıvestigating how a wave component $\exp(-\alpha k^2 t)\exp(ikx)$ is treated by the
umerical scheme. It appears that such wave components are also solutions of
ıe schemes, but the damping factor $\exp(-\alpha k^2 t)$ varies among the schemes. To
ıse the forthcoming algebra, we write the damping factor as A^n. The exact
mplification factor corresponding to A is $A_{\mathrm{e}} = \exp(-\alpha k^2 \Delta t)$.

.3 Analysis of the finite difference schemes

Ve have seen that a general solution of the diffusion equation can be built as a
near combination of basic components

$$e^{-\alpha k^2 t} e^{ikx}\,.$$

A fundamental question is whether such components are also solution
finite difference schemes. This is indeed the case, but the amplitude exp
might be modified (which also happens when solving the ODE cou
$u' = -\alpha u$). We therefore look for numerical solutions of the form

$$u_q^n = A^n e^{ikq\Delta x} = A^n e^{ikx},$$

where the amplification factor A must be determined by inserting the co
into an actual scheme.

Stability. The exact amplification factor is $A_{\mathrm{e}} = \exp(-\alpha^2 k^2 \Delta t)$. W
therefore require $|A| < 1$ to have a decaying numerical solution as
$-1 \leq A < 0$, A^n will change sign from time level to time level, and we ge
non-physical oscillations in the numerical solutions that are not presen
exact solution.

Accuracy. To determine how accurately a finite difference scheme tr
wave component (53), we see that the basic deviation from the exact so
reflected in how well A^n approximates A_{e}^n, or how well A approximates

2.4 Analysis of the Forward Euler scheme

The Forward Euler finite difference scheme for $u_t = \alpha u_{xx}$ can be writte

$$[D_t^+ u = \alpha D_x D_x u]_q^n\,.$$

Inserting a wave component (53) in the scheme demands calculating th

$$e^{ikq\Delta x}[D_t^+ A]^n = e^{ikq\Delta x} A^n \frac{A-1}{\Delta t},$$

and

$$A^n D_x D_x [e^{ikx}]_q = A^n \left(-e^{ikq\Delta x} \frac{4}{\Delta x^2} \sin^2\left(\frac{k\Delta x}{2}\right)\right)\,.$$

Inserting these terms in the discrete equation and dividing by $A^n e^{ikq\Delta x}$

$$\frac{A-1}{\Delta t} = -\alpha \frac{4}{\Delta x^2} \sin^2\left(\frac{k\Delta x}{2}\right),$$

and consequently

$$A = 1 - 4F_o \sin^2\left(\frac{k\Delta x}{2}\right),$$

where

$$F_o = \frac{\alpha \Delta t}{\Delta x^2}$$

the *numerical Fourier number*. The complete numerical solution is then

$$u_q^n = \left(1 - 4F_o \sin^2\left(\frac{k\Delta x}{2}\right)\right)^n e^{ikq\Delta x}\,. \tag{56}$$

tability. We easily see that $A \leq 1$. However, the A can be less than -1, hich will lead to growth of a numerical wave component. The criterion $A \geq -1$ nplies

$$4F_o \sin^2(p/2) \leq 2\,.$$

he worst case is when $\sin^2(p/2) = 1$, so a sufficient criterion for stability is

$$F_o \leq \frac{1}{2}, \tag{57}$$

r expressed as a condition on Δt:

$$\Delta t \leq \frac{\Delta x^2}{2\alpha}\,. \tag{58}$$

ote that halving the spatial mesh size, $\Delta x \to \frac{1}{2}\Delta x$, requires Δt to be reduced y a factor of 1/4. The method hence becomes very expensive for fine spatial ieshes.

ccuracy. Since A is expressed in terms of F_o and the parameter we now call $= k\Delta x/2$, we also express A_e by F_o and p:

$$A_\mathrm{e} = \exp\left(-\alpha k^2 \Delta t\right) = \exp\left(-4F_o p^2\right).$$

omputing the Taylor series expansion of A/A_e in terms of F_o can easily be one with aid of `sympy`:

```
def A_exact(Fo, p):
    return exp(-4*Fo*p**2)

def A_FE(Fo, p):
    return 1 - 4*Fo*sin(p)**2

from sympy import *
Fo, p = symbols('Fo p')
A_err_FE = A_FE(Fo, p)/A_exact(Fo, p)
print A_err_FE.series(Fo, 0, 6)
```

he result is

$$\frac{A}{A_\mathrm{e}} = 1 - 4F_o \sin^2 p + 2F_o p^2 - 16F_o^2 p^2 \sin^2 p + 8F_o^2 p^4 + \cdots$$

ecalling that $F_o = \alpha\Delta t/\Delta x$, $p = k\Delta x/2$, and that $\sin^2 p \leq 1$, we realize that ie dominating error terms are at most

$$1 - 4\alpha\frac{\Delta t}{\Delta x^2} + \alpha\Delta t - 4\alpha^2\Delta t^2 + \alpha^2\Delta t^2\Delta x^2 + \cdots\,.$$

2.5 Analysis of the Backward Euler scheme

Discretizing $u_t = \alpha u_{xx}$ by a Backward Euler scheme,

$$[D_t^- u = \alpha D_x D_x u]_q^n,$$

and inserting a wave component (53), leads to calculations similar t arising from the Forward Euler scheme, but since

$$e^{ikq\Delta x}[D_t^- A]^n = A^n e^{ikq\Delta x}\frac{1 - A^{-1}}{\Delta t},$$

we get

$$\frac{1 - A^{-1}}{\Delta t} = -\alpha\frac{4}{\Delta x^2}\sin^2\left(\frac{k\Delta x}{2}\right),$$

and then

$$A = \left(1 + 4F_o \sin^2 p\right)^{-1}\,.$$

The complete numerical solution can be written

$$u_q^n = \left(1 + 4F_o \sin^2 p\right)^{-n} e^{ikq\Delta x}\,.$$

Stability. We see from (59) that $0 < A < 1$, which means that all nu wave components are stable and non-oscillatory for any $\Delta t > 0$.

2.6 Analysis of the Crank-Nicolson scheme

The Crank-Nicolson scheme can be written as

$$[D_t u = \alpha D_x D_x \overline{u}^x]_q^{n+\frac{1}{2}},$$

or

$$[D_t u]_q^{n+\frac{1}{2}} = \frac{1}{2}\alpha\left([D_x D_x u]_q^n + [D_x D_x u]_q^{n+1}\right)\,.$$

Inserting (53) in the time derivative approximation leads to

$$[D_t A^n e^{ikq\Delta x}]^{n+\frac{1}{2}} = A^{n+\frac{1}{2}} e^{ikq\Delta x}\frac{A^{\frac{1}{2}} - A^{-\frac{1}{2}}}{\Delta t} = A^n e^{ikq\Delta x}\frac{A - 1}{\Delta t}\,.$$

Inserting (53) in the other terms and dividing by $A^n e^{ikq\Delta x}$ gives the re

$$\frac{A - 1}{\Delta t} = -\frac{1}{2}\alpha\frac{4}{\Delta x^2}\sin^2\left(\frac{k\Delta x}{2}\right)(1 + A),$$

and after some more algebra,

$$A = \frac{1 - 2F_o \sin^2 p}{1 + 2F_o \sin^2 p}\,.$$

he exact numerical solution is hence

$$u_q^n = \left(\frac{1 - 2F_o \sin^2 p}{1 + 2F_o \sin^2 p}\right)^n e^{ikp\Delta x}\,. \tag{62}$$

tability. The criteria $A > -1$ and $A < 1$ are fulfilled for any $\Delta t > 0$.

.7 Summary of accuracy of amplification factors

Ve can plot the various amplification factors against $p = k\Delta x/2$ for different ıoices of the F_o parameter. Figures 2, 3, and 4 show how long and small aves are damped by the various schemes compared to the exact damping. As ɔng as all schemes are stable, the amplification factor is positive, except for rank-Nicolson when $F_o > 0.5$.

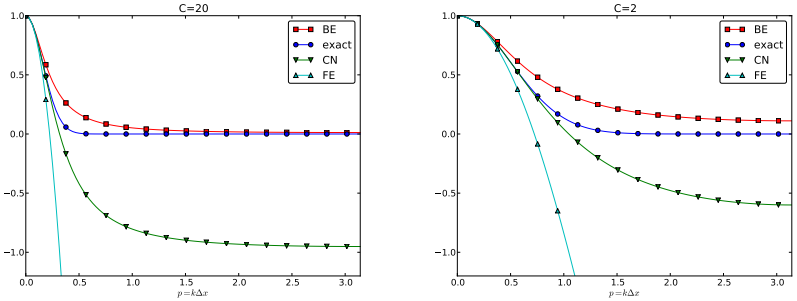
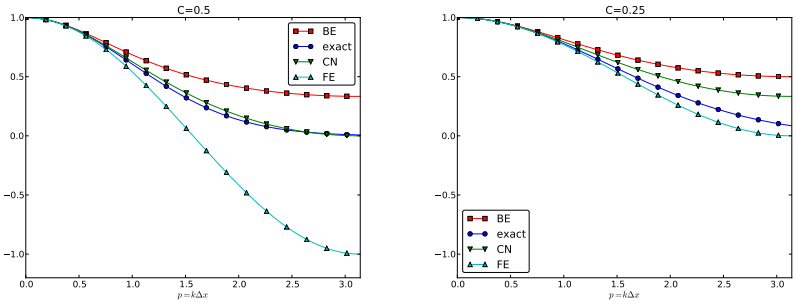


Figure 2: Amplification factors for large time steps.



igure 3: Amplification factors for time steps around the Forward Euler stability mit.

The effect of negative amplification factors is that A^n changes sign from one me level to the next, thereby giving rise to oscillations in time in an animation f the solution. We see from Figure 2 that for $F_o = 20$, waves with $p \geq \pi/2$ ndergo a damping close to -1, which means that the amplitude does not decay

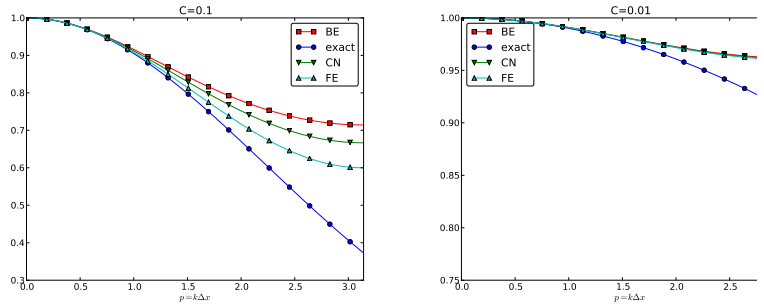


Figure 4: Amplification factors for small time steps.

and that the wave component jumps up and down in time. For $F_o = 2$ a damping of a factor of 0.5 from one time level to the next, which is ver smaller than the exact damping. Short waves will therefore fail to be eff dampened. These waves will manifest themselves as high frequency osc noise in the solution.

A value $p = \pi/4$ corresponds to four mesh points per wave length while $p = \pi/2$ implies only two points per wave length, which is the s number of points we can have to represent the wave on the mesh.

To demonstrate the oscillatory behavior of the Crank-Nicolson sch choose an initial condition that leads to short waves with significant am A discontinuous $I(x)$ will in particular serve this purpose.

Run $F_o =$ .....

Exercise 1: Use an analytical solution to formulate test

This exercise explores the exact solution (48). We shall formulate a d problem in half of the domain for half of the Gaussian pulse. Then v investigate the impact of using an incorrect boundary condition, whic general cases often are forced due if the solution needs to pass throug boundaries undisturbed.

a) The solution (48) is seen to be symmetric at $x = c$, because $\partial u/$ always vanishes for $x = c$. Use this property to formulate a complet boundary value problem in 1D involving the diffusion equation $u_t =$ $[0, L]$ with $u_x(0, t) = 0$ and $u(L, t)$ known.

b) Use the exact solution to set up a convergence rate test for an implem of the problem. Investigate if a one-sided difference for $u_x(0, t)$, say u destroys the second-order accuracy in space.

c) Imagine that we want to solve the problem numerically on $[0, L]$, bu not know the exact solution and cannot of that reason assign a correct I condition at $x = L$. One idea is to simply set $u(L, t) = 0$ since this

n accurate approximation before the diffused pulse reaches $x = L$ and even ıereafter it might be a satisfactory condition. Let u_e be the exact solution nd let u be the solution of $u_t = \alpha u_{xx}$ with an initial Gaussian pulse and the oundary conditions $u_x(0,t) = u(L,t) = 0$. Derive a diffusion problem for ıe error $e = u_e - u$. Solve this problem numerically using an exact Dirichlet ɔndition at $x = L$. Animate the evolution of the error and make a curve plot of ıe error measure

$$E(t) = \sqrt{\frac{\int_0^L e^2 dx}{\int_0^L u dx}}.$$

ɜ this a suitable error measure for the present problem?

) Instead of using $u(L,t) = 0$ as approximate boundary condition for letting the iffused Gaussian pulse out of our finite domain, one may try $u_x(L,t) = 0$ since ıe solution for large t is quite flat. Argue that this condition gives a completely rong asymptotic solution as $t \to 0$. To do this, integrate the diffusion equation om 0 to L, integrate u_{xx} by parts (or use Gauss' divergence theorem in 1D) to rrive at the important property

$$\frac{d}{dt}\int_0^L u(x,t)dx = 0,$$

nplying that $\int_0^L u dx$ must be constant in time, and therefore

$$\int_0^L u(x,t)dx = \int_0^L I(x)dx\,.$$

he integral of the initial pulse is 1.

) Another idea for an artificial boundary condition at $x = L$ is to use a cooling ıw

$$-\alpha u_x = q(u - u_S), \tag{63}$$

here q is an unknown heat transfer coefficient and u_S is the surrounding ɜmperature in the medium outside of $[0, L]$. (Note that arguing that u_S is pproximately $u(L,t)$ gives the $u_x = 0$ condition from the previous subexercise ıat is qualitatively wrong for large t.) Develop a diffusion problem for the error ı the solution using (63) as boundary condition. Assume one can take $u_S = 0$ ɔutside the domain" as $u \to 0$ for $x \to \infty$. Find a function $q = q(t)$ such that ıe exact solution obeys the condition (63). Test some constant values of q nd animate how the corresponding error function behaves. Also compute $E(t)$ ırves as suggested in subexercise b).
ilename: `diffu_symmetric_gaussian.py`.

Exercise 2: Use an analytical solution to formulate test

Generalize (48) to multi dimensions by assuming that one-dimensional s can be multiplied to solve $u_t = \alpha\nabla^2 u$. Use this solution to formulate a case where the peak of the Gaussian is at the origin and where the dom rectangle in the first quadrant. Use symmetry boundary conditions ∂ 0 whereever possible, and use exact Dirichlet conditions on the rei boundaries. Filename: `diffu_symmetric_gaussian_2D.pdf`.

Exercise 3: Examine stability of a diffusion model v source term

Consider a diffusion equation with a linear u term:

$$u_t = \alpha u_{xx} + \beta u\,.$$

a) Derive in detail a Forward Euler scheme, a Backward Euler scheme Crank-Nicolson for this type of diffusion model. Thereafter, formulate to summarize the three schemes.

b) Assume a solution like (49) and find the relation between a, k, α, a

c) Calculate the stability of the Forward Euler scheme. Design nu experiments to confirm the results.

d) Repeat c) for the Backward Euler scheme.

e) Repeat c) for the Crank-Nicolson scheme.

f) How does the extra term bu impact the accuracy of the three schem

Hint. Compare the numerical and exact amplification factors, either ir or by Taylor series expansion (or both).
Filename: `diffu_stab_uterm.pdf`.

3 Diffusion in heterogeneous media

Diffusion in heterogeneous media will normally imply a non-constant d coefficient $\alpha = \alpha(x)$. A 1D diffusion model with such a variable d coefficient reads

$$\begin{aligned}
\frac{\partial u}{\partial t} &= \frac{\partial}{\partial x}\left(\alpha(x)\frac{\partial u}{\partial x^2}\right), \quad x \in (0,L),\ t \in (0,T] \\
u(x,0) &= I(x), && x \in [0,L] \\
u(0,t) &= U_L, && t > 0, \\
u(L,t) &= U_0, && t > 0\,.
\end{aligned}$$

short form of the diffusion equation with variable coefficients is $u_t = (\alpha u_x)_x$.

.1 Stationary solution

s $t \to \infty$, the solution of the above problem will approach a stationary limit here $\partial u/\partial t = 0$. The governing equation is then

$$\frac{d}{dx}\left(\alpha \frac{du}{dx}\right) = 0, \tag{68}$$

ith boundary conditions $u(0) = U_0$ and $u(L) = u_L$. It is possible to obtain an xact solution of (68) for any α. Integrating twice and applying the boundary onditions to determine the integration constants gives

$$u(x) = U_0 + (U_L - U_0)\frac{\int_0^x (\alpha(\xi))^{-1} d\xi}{\int_0^L (\alpha(\xi))^{-1} d\xi}. \tag{69}$$

.2 Piecewise constant medium

onsider a medium built of M layers. The boundaries between the layers are enoted by $b_0, \ldots, b_M$, where $b_0 = 0$ and $b_M = L$. If the material in each layer otentially differs from the others, but is otherwise constant, we can express α s a *piecewise constant function* according to

$$\alpha(x) = \begin{cases} \alpha_0, & b_0 \leq x < b_1, \\ \vdots & \\ \alpha_i, & b_i \leq x < b_{i+1}, \\ \vdots & \\ \alpha_0, & b_{M-1} \leq x \leq b_M. \end{cases} \tag{70}$$

The exact solution (69) in case of such a piecewise constant α function is easy o derive. Assume that x is in the m-th layer: $x \in [b_m, b_{m+1}]$. In the integral $\int_0^x (a(\xi))^{-1} d\xi$ we must integrate through the first $m-1$ layers and then add the ontribution from the remaining part $x - b_m$ into the m-th layer:

$$u(x) = U_0 + (U_L - U_0)\frac{\sum_{j=0}^{m-1}(b_{j+1} - b_j)/\alpha(b_j) + (x - b_m)/\alpha(b_m)}{\sum_{j=0}^{M-1}(b_{j+1} - b_j)/\alpha(b_j)} \tag{71}$$

emark. It may sound strange to have a discontinuous α in a differential quation where one is to differentiate, but a discontinuous α is compensated by discontinuous u_x such that αu_x is continues and therefore can be differentiated s $(\alpha u_x)_x$.

3.3 Implementation

Programming with piecewise function definition quickly becomes cumb as the most naive approach is to test for which interval x lies, and th evaluating a formula like (71). In Python, vectorized expressions m to speed up the computations. The convenience classes `PiecewiseCo` and `IntegratedPiecewiseConstant` were made to simplify programmi functions like (3.2) and expressions like (71). These utilities not only re piecewise constant functions, but also *smoothed* versions of them wh discontinuities can be smoothed out in a controlled fashion. This is advan in many computational contexts (although seldom for pure finite di computations of the solution u).

The `PiecewiseConstant` class is created by sending in the doma 2-tuple or 2-list and a `data` object describing the boundaries $b_0, \ldots, b_M$ corresponding function values $\alpha_0, \ldots, \alpha_{M-1}$. More precisely, `data` is a list, where `data[i][0]` holds b_i and `data[i][1]` holds the correspondi α_i, for $i = 0, \ldots, M-1$. Given b_i and α_i in arrays `b` and `a`, it is easy to the nested list `data`.

In our application, we want to represent α and $1/\alpha$ as piecewise c function, in addition to the $u(x)$ function which involves the integrals of class creating the functions we need and a method for evaluating u, can form

```
class SerialLayers:
    """
    b: coordinates of boundaries of layers, b[0] is left boundary
    and b[-1] is right boundary of the domain [0,L].
    a: values of the functions in each layer (len(a) = len(b)-1).
    U_0: u(x) value at left boundary x=0=b[0].
    U_L: u(x) value at right boundary x=L=b[0].
    """

    def __init__(self, a, b, U_0, U_L, eps=0):
        self.a, self.b = np.asarray(a), np.asarray(b)
        self.eps = eps  # smoothing parameter for smoothed a
        self.U_0, self.U_L = U_0, U_L

        a_data = [[bi, ai] for bi, ai in zip(self.b, self.a)]
        domain = [b[0], b[-1]]
        self.a_func = PiecewiseConstant(domain, a_data, eps)

        # inv_a = 1/a is needed in formulas
        inv_a_data = [[bi, 1./ai] for bi, ai in zip(self.b, self.
        self.inv_a_func = \
             PiecewiseConstant(domain, inv_a_data, eps)
        self.integral_of_inv_a_func = \
             IntegratedPiecewiseConstant(domain, inv_a_data, eps)
        # Denominator in the exact formula is constant
        self.inv_a_0L = self.integral_of_inv_a_func(b[-1])

    def __call__(self, x):
        solution = self.U_0 + (self.U_L-self.U_0)*\
                   self.integral_of_inv_a_func(x)/self.inv_a_0L
        return solution
```

A visualization method is also convenient to have. Below we plot $u(x)$ long with $\alpha(x)$ (which works well as long as $\max \alpha(x)$ is of the same size as $\max u = \max(U_0, U_L)$).

```
class SerialLayers:
    ...

    def plot(self):
        x, y_a = self.a_func.plot()
        x = np.asarray(x); y_a = np.asarray(y_a)
        y_u = self.u_exact(x)
        import matplotlib.pyplot as plt
        plt.figure()
        plt.plot(x, y_u, 'b')
        plt.hold('on')  # Matlab style
        plt.plot(x, y_a, 'r')
        ymin = -0.1
        ymax = 1.2*max(y_u.max(), y_a.max())
        plt.axis([x[0], x[-1], ymin, ymax])
        plt.legend(['solution $u$', 'coefficient $a$'], loc='upper left')
        if self.eps > 0:
            plt.title('Smoothing eps: %s' % self.eps)
        plt.savefig('tmp.pdf')
        plt.savefig('tmp.png')
        plt.show()
```

Figure 5 shows the case where

```
= [0, 0.25, 0.5, 1]   # material boundaries
= [0.2, 0.4, 4]       # material values
_0 = 0.5;  U_L = 5    # boundary conditions
```

By adding the `eps` parameter to the constructor of the `SerialLayers` class, e can experiment with smoothed versions of α and see the (small) impact on u. igure 6 shows the result.

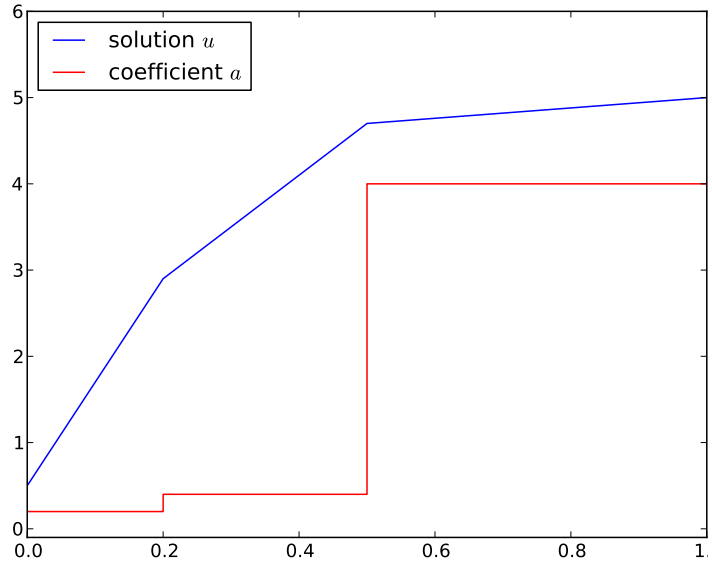
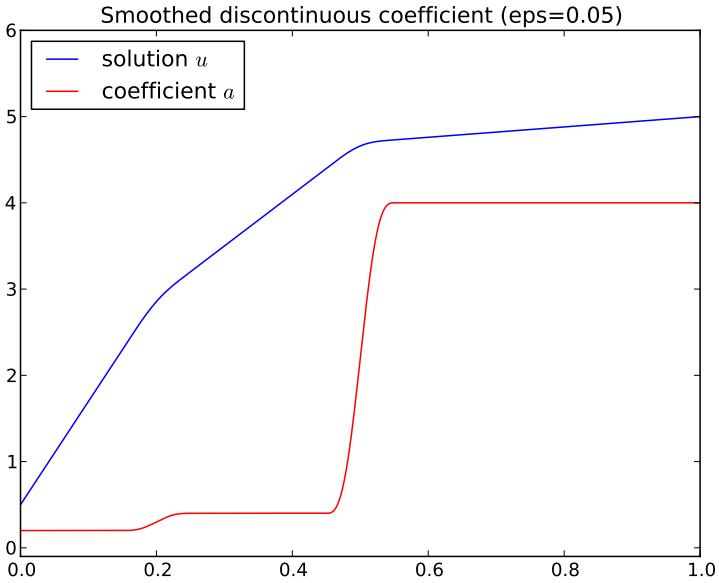


Figure 5: Solution of the stationary diffusion equation correspondi piecewise constant diffusion coefficient.



igure 6: Solution of the stationary diffusion equation corresponding to a *noothed* piecewise constant diffusion coefficient.

4 Exercises

Exercise 4: Stabilizing the Crank-Nicolson method by nacher time stepping

It is well known that the Crank-Nicolson method may give rise to non- oscillations in the solution of diffusion equations if the initial data exhibi (see Section 2.6). Rannacher [1] suggested a stabilizing technique consi using the Backward Euler scheme for the first two time steps with ste $\frac{1}{2}\Delta t$. One can generalize this idea to taking $2m$ time steps of size $\frac{1}{2}\Delta t$ Backward Euler method and then continuing with the Crank-Nicolson which is of second-order in time. The idea is that the high frequencie initial solution are quickly damped out, and the Backward Euler schem these high frequencies correctly. Thereafter, the high frequency conten solution is gone and the Crank-Nicolson method will do well.

Test this idea for $m = 1, 2, 3$ on a diffusion problem with a discon initial condition. Measure the convergence rate using the solution (45) boundary conditions (46)-(47) for t values such that the conditions ar vicinity of ± 1. For example, $t < 5a1.6 \cdot 10^{-2}$ makes the solution diffusio step to almost a straight line. The program `diffu_erf_sol.py` shows compute the analytical solution.

Project 5: Energy estimates for diffusion problems

This project concerns so-called *energy estimates* for diffusion problems t be used for qualitative analytical insight and for verification of impleme

a) We start with a 1D homogeneous diffusion equation with zero I conditions:

$$
\begin{aligned}
u_t &= \alpha u_x x, && x \in \Omega = (0, L),\ t \in (0, T], \\
u(0, t) = u(L, t) &= 0, && t \in (0, T], \\
u(x, 0) &= I(x), && x \in [0, L]\,.
\end{aligned}
$$

The energy estimate for this problem reads

$$
||u||_{L^2} \leq ||I||_{L^2},
$$

where the $||\cdot||_{L^2}$ norm is defined by

$$
||g||_{L^2} = \sqrt{\int_0^L g^2 dx}\,.
$$

The quantify $||u||_{L^2}$ or $\frac{1}{2}||u||_{L^2}$ is known as the *energy* of the solution, alt is not the physical energy of the system. A mathematical tradition has int the notion *energy* in this context.

The estimate (75) says that the "size of u" never exceeds that of the initial ɔndition, or more equivalently, that the area under the u curve decreases with me.

To show (75), multiply the PDE by u and integrate from 0 to L. Use that u_t can be expressed as the time derivative of u^2 and that u_xxu can integrated y parts to form an integrand u_x^2. Show that the time derivative of $||u||_{L^2}^2$ must e less than or equal to zero. Integrate this expression and derive (75).

) Now we address a slightly different problem,

$$u_t = \alpha u_x x + f(x,t), \qquad x \in \Omega = (0,L),\ t \in (0,T], \tag{77}$$

$$u(0,t) = u(L,t) = 0, \qquad t \in (0,T], \tag{78}$$

$$u(x,0) = 0, \qquad x \in [0,L]\,. \tag{79}$$

he associated energy estimate is

$$||u||_{L^2} \leq ||f||_{L^2}\,. \tag{80}$$

This result is more difficult to derive.)

Now consider the compound problem with an initial condition $I(x)$ and a ght-hand side $f(x,t)$:

$$u_t = \alpha u_x x + f(x,t), \qquad x \in \Omega = (0,L),\ t \in (0,T], \tag{81}$$

$$u(0,t) = u(L,t) = 0, \qquad t \in (0,T], \tag{82}$$

$$u(x,0) = I(x), \qquad x \in [0,L]\,. \tag{83}$$

how that if w_1 fulfills (72)-(74) and w_2 fulfills (77)-(79), then $u = w_1 + w_2$ is ıe solution of (81)-(83). Using the triangle inequality for norms,

$$||a+b|| \leq ||a|| + ||b||,$$

ıow that the energy estimate for (81)-(83) becomes

$$||u||_{L^2} \leq ||I||_{L^2} + ||f||_{L^2}\,. \tag{84}$$

) One application of (84) is to prove uniqueness of the solution. Suppose u_1 ıd u_2 both fulfill (81)-(83). Show that $u = u_1 - u_2$ then fulfills (81)-(83) with $= 0$ and $I = 0$. Use (84) to deduce that the energy must be zero for all times ıd therefore that $u_1 = u_2$, which proves that the solution is unique.

) Generalize (84) to a 2D/3D diffusion equation $u_t = \nabla\cdot(\alpha\nabla u)$ for $x \in \Omega$.

Hint. Use integration by parts in multi dimensions:

$$\int_\Omega u\nabla\cdot(\alpha\nabla u)\,\mathrm{d}x = -\int_\Omega \alpha\nabla u\cdot\nabla u\,\mathrm{d}x + \int_{\partial\Omega} u\alpha\frac{\partial u}{\partial n},$$

here $\frac{\partial u}{\partial n} = \boldsymbol{n}\cdot\nabla u$, $\boldsymbol{n}$ being the outward unit normal to the boundary $\partial\Omega$ of the omain Ω.

e) Now we also consider the multi-dimensional PDE $u_t = \nabla\cdot(\alpha\nabla u)$. Ir both sides over Ω and use Gauss' divergence theorem, $\int_\Omega \nabla\cdot\boldsymbol{q}\,\mathrm{d}x = \int_{\partial\Omega}$ for a vector field $\boldsymbol{q}$. Show that if we have homogeneous Neumann condi the boundary, $\partial u/\partial n = 0$, area under the u surface remains constant and

$$\int_\Omega u\,\mathrm{d}x = \int_\Omega I\,\mathrm{d}x\,.$$

f) Establish a code in 1D, 2D, or 3D that can solve a diffusion equatior source term f, initial condition I, and zero Dirichlet or Neumann condi the whole boundary.

We can use (84) and (85) as a partial verification of the code. Choo functions f and I and check that (84) is obeyed at any time when zero I conditions are used. Iterate over the same I functions and check that fulfilled when using zero Neumann conditions.

g) Make a list of some possible bugs in the code, such as indexing e arrays, failure to set the correct boundary conditions, evaluation of a te wrong time level, and similar. For each of the bugs, see if the verificati from the previous subexercise pass or fail. This investigation shows how the energy estimates and the estimate (85) are for pointing out error implementation.

Filename: `diffu_energy.pdf`.

References

[1] R. Rannacher. Finite element solution of diffusion problems with i data. *Numerische Mathematik*, 43:309–327, 1984.

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